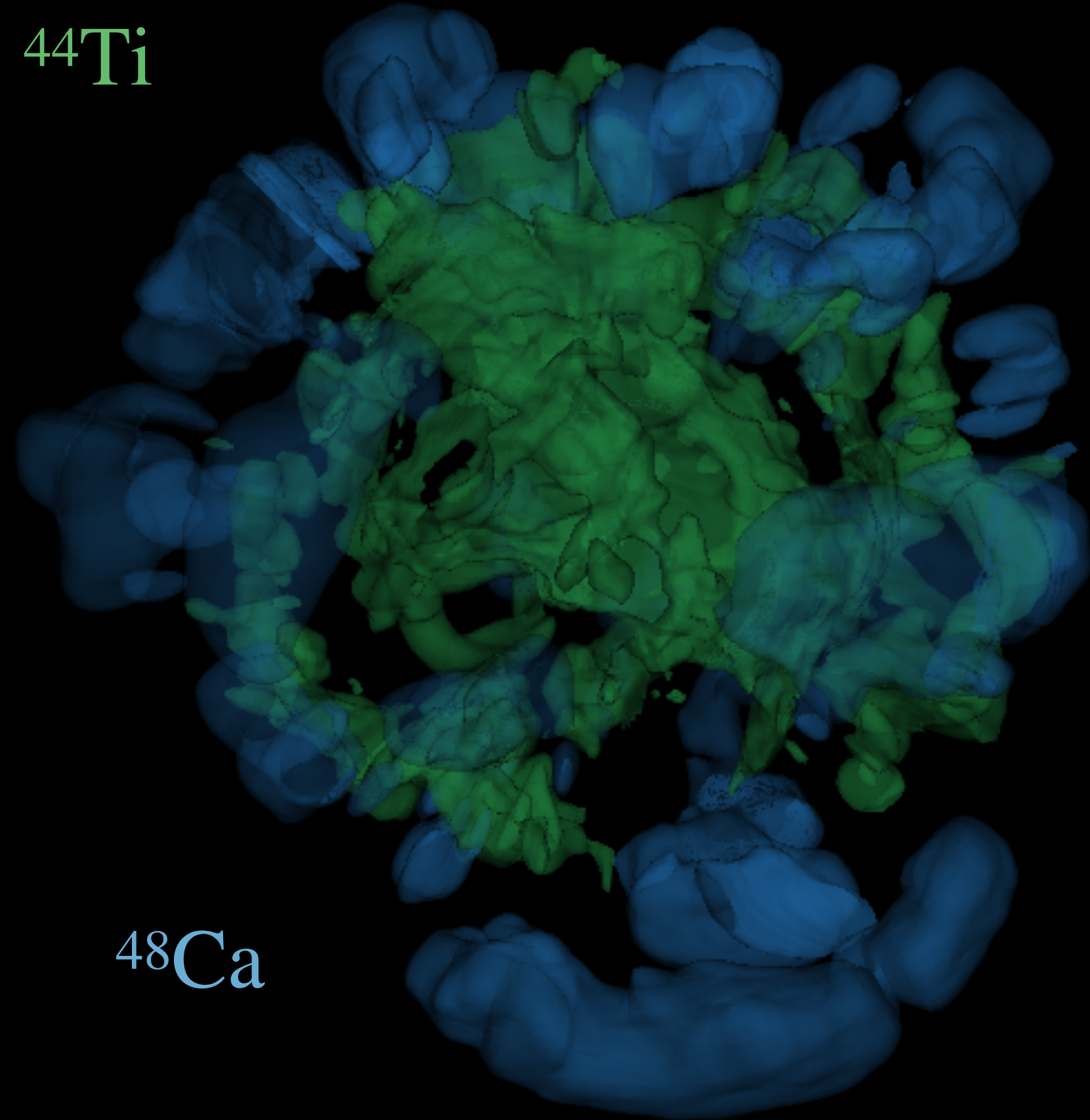


# OPPORTUNITIES & NEEDS FOR

02560.xmf

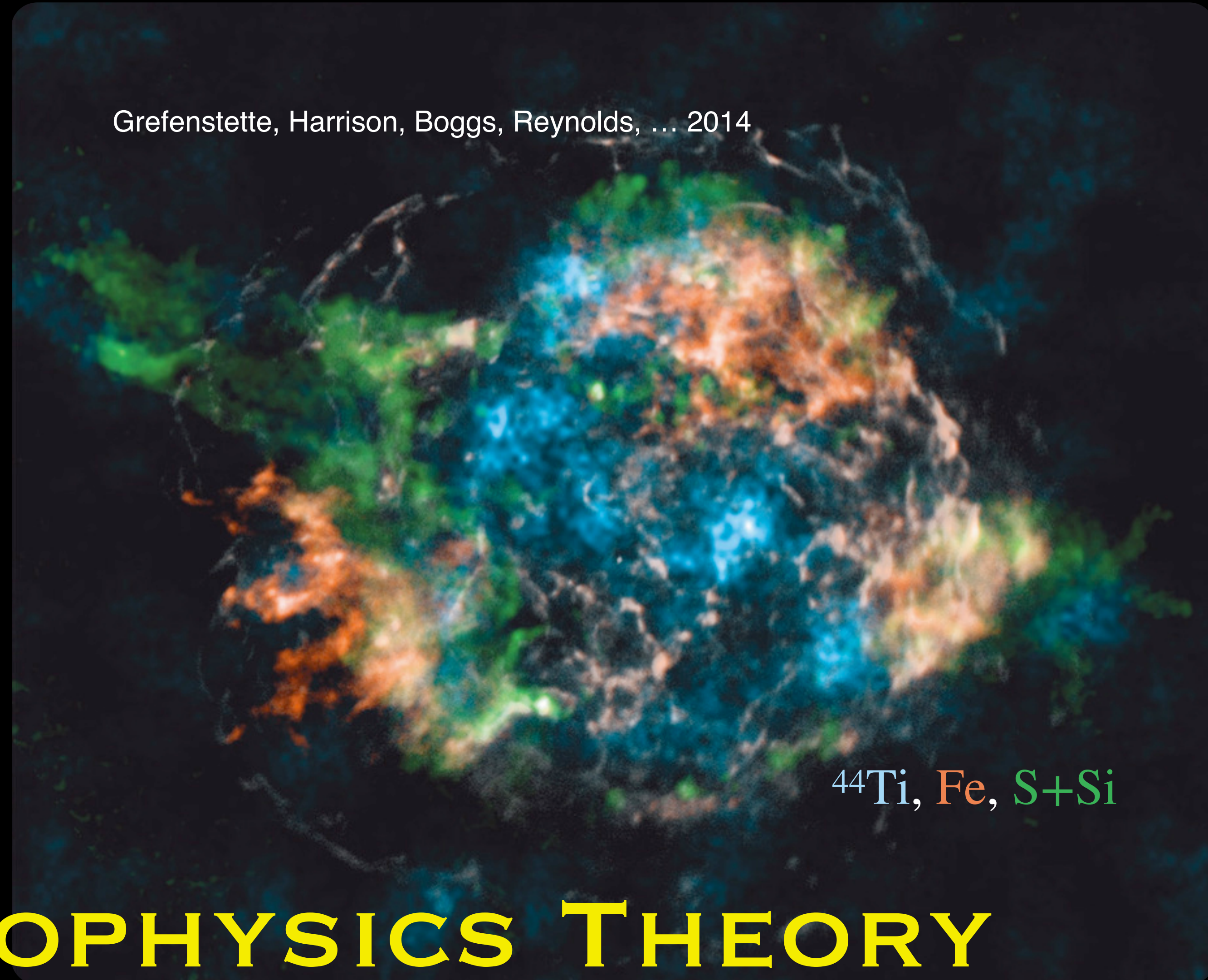
$^{44}\text{Ti}$



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$^{48}\text{Ca}$

Grefenstette, Harrison, Boggs, Reynolds, ... 2014



$^{44}\text{Ti}$ , Fe, S+Si

x

# NUCLEAR ASTROPHYSICS THEORY

William Raphael Hix (ORNL/U. Tennessee)

# What we know (thanks to simulations)

Have a good modelling of the **inspiral** stage and know that **tidal deformability** leads to measurable changes in the GW signal which we can constrain.

Have good understanding of **post-merger** emission: **GW spectroscopy** is possible via peaks and universal relations

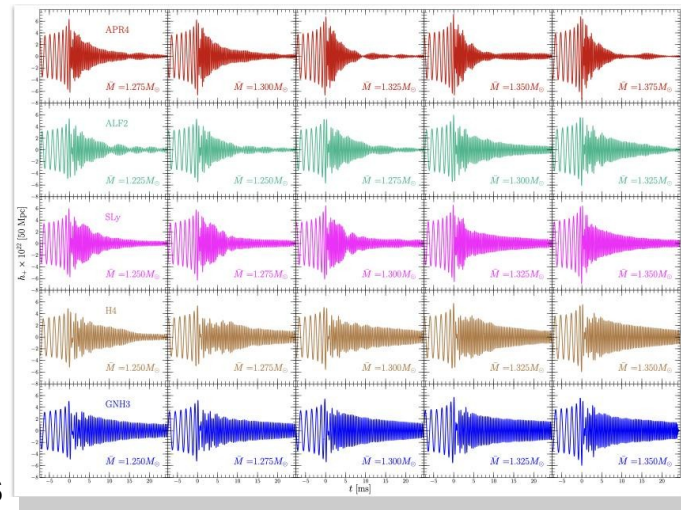
Have a poor understanding of role of **magnetic fields** in determining **jet launching** and **propagation**.

Have an incomplete understanding of the appearance of **phase transition to quark matter**

Have a reasonable understanding of role of **neutrinos** in **mass ejection** and its “**chemical**” evolution

Have a limited understanding of **r-process nucleosynthesis** and production of heavy elements.

Have a poor understanding of generation of **kilonova** emission and of the **radiative transport** in ejected matter



# What we need to know

What is the precise impact of **tidal deformability** and hence of **EOS** on the inspiral waveforms?

What is the **long-term** (100+ ms) dynamics of merger **remnant** and its **lifetime**?

What is the amount of **mass ejected** both **dynamically** and **secularly**?

How important is the role played by **neutrinos** in **mass ejection** and lifetime of HMNS?

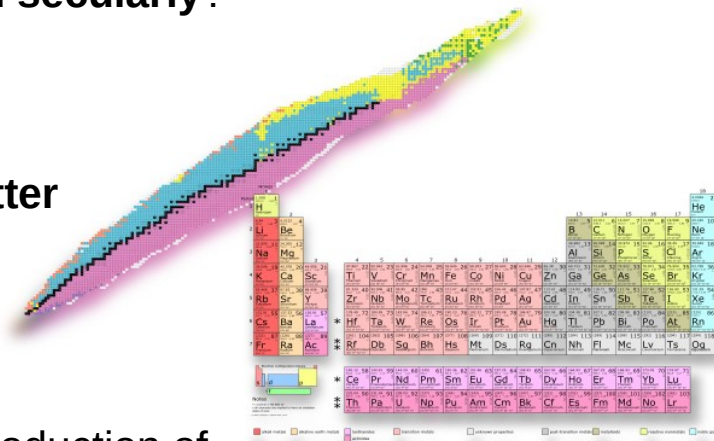
What are the signatures of **phase transitions** to **quark matter** or of other states (CFL phase)?

How is a relativistic jet launched in the merger of magnetized BNSs?

What are the details of **r-process nucleosynthesis** and production of heavy elements?

How can we extract information on **r-process nucleosynthesis** from astronomical observations?

How can we extract precise information on **chemical abundances** from kilonova lightcurves?



# NS Mergers Required Developments

General requirements:

- Codes capable of leveraging exascale machines
  - Simulations will require higher dimensions, higher resolution, longer evolutions, and the evolution of many more variables!
  - Merger -> Post-merger -> Outflow evolution and r-process nucleosynthesis -> Kilonova modeling and synchrotron emission need to be modeled self-consistently!
- Development of accurate and computationally efficient algorithm for
  - Generation of high-accuracy GW templates (+methods to choose template locations)
  - Neutrino transport and neutrino matter interactions (crucial for r-process)
  - Magnetic fields (growth and saturation of instabilities, turbulence, **dynamo, jets**)
  - Out-of-equilibrium nuclear reactions (on-the-fly nuclear reaction networks?)
  - Non-ideal physics? (resistivity, viscosity, conduction)
- Improved collaborations with nuclear physicists
  - “Realistic” equations of state usable in high-accuracy simulations
  - Neutrino-matter interactions
  - (Simplified) nuclear reaction networks

# R-process What do we need from the nuclear physics community?

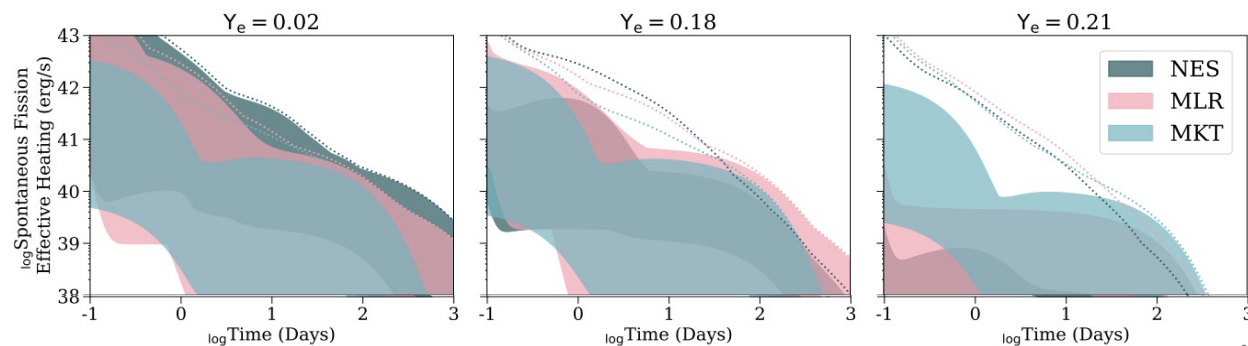
## *Some specific physics needs*

### Neutron capture

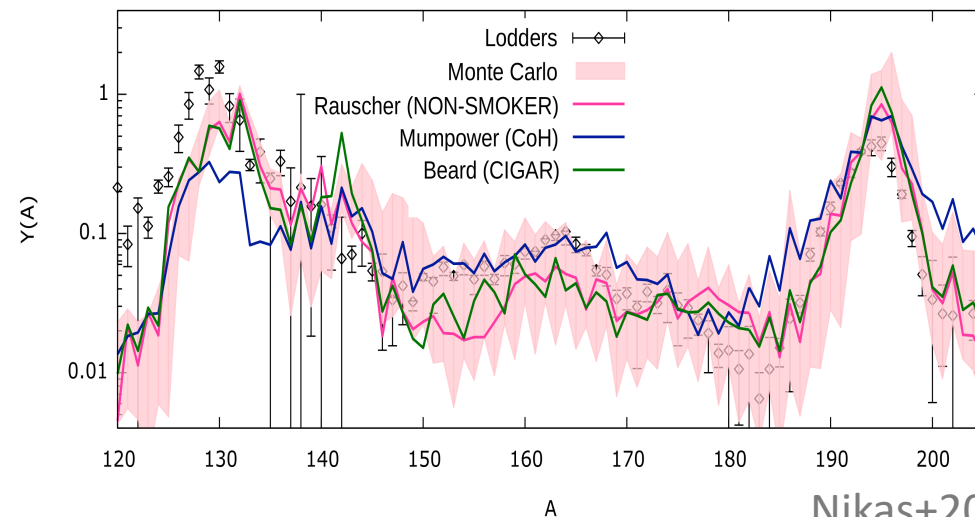
- \*only have direct measurements on stable nuclei and indirect measurements a few neutrons from stability
- \*theoretical rates can vary by an order of magnitude or more

### $\beta$ -decay

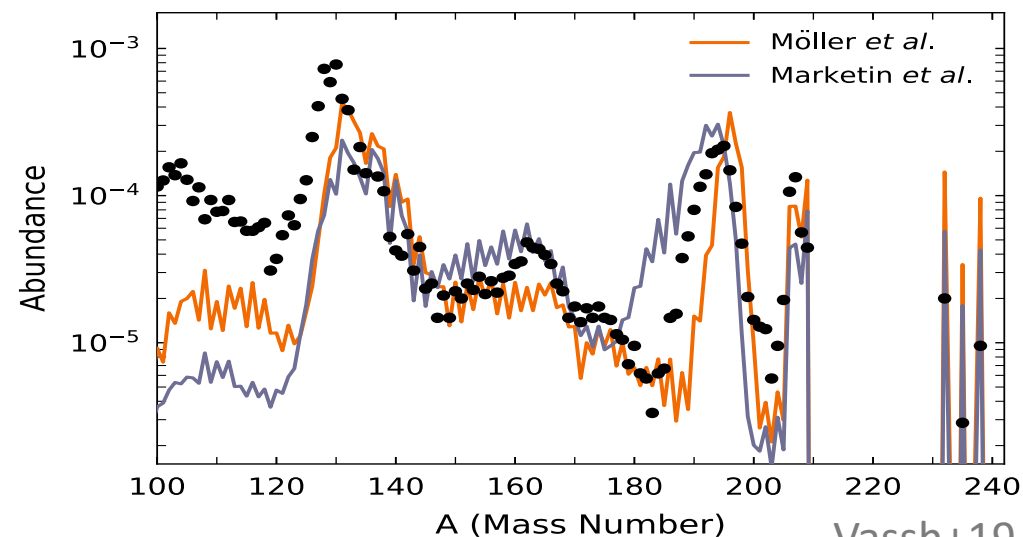
- \**rates*: studies find to have a particularly big impact on the abundances of third peak (N=126) and the actinides
- \**neutron emission probabilities*: especially important at times when *r* process in most n-rich regions; shape abundances locally and provide a source of extra neutrons
- \* $\beta$ -decay heating for light curves and  $\beta$  MeV gamma spectra are crucial elements to interpret EM signals from events and remnants



Lund+22



Nikas+20



Vassh+19

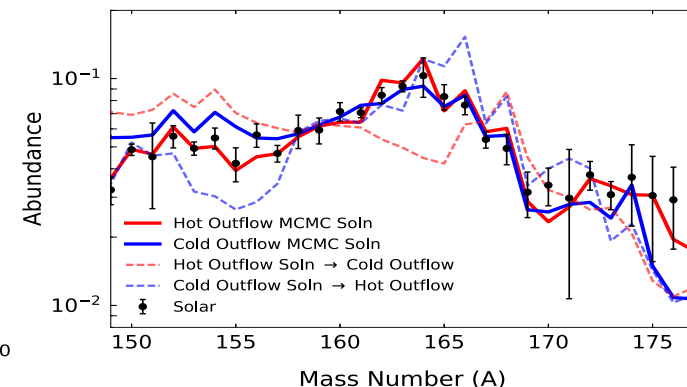
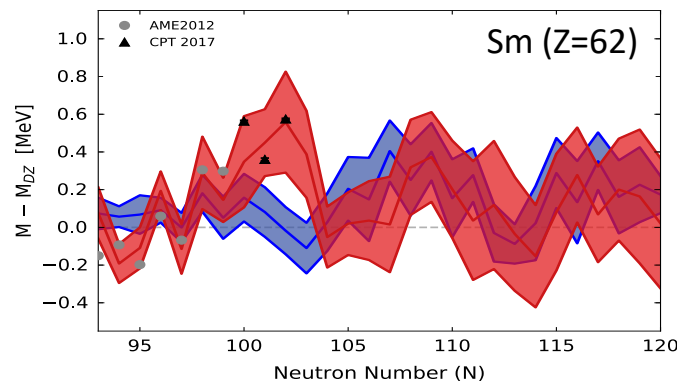
# R-process What do we need from the nuclear physics community?

## Some specific physics needs

### Nuclear masses

Enter predictions both directly and indirectly:

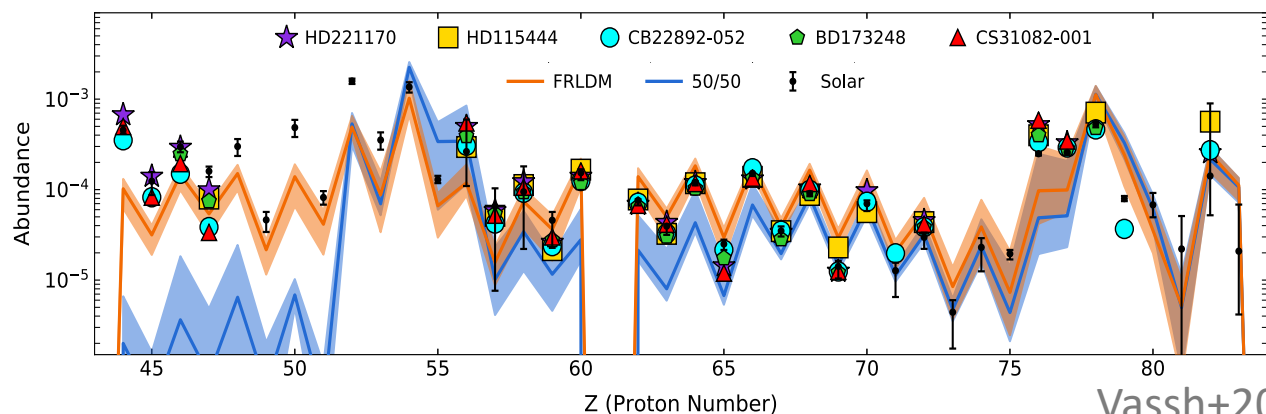
- \*Q-values for  $\beta$ -decay rates / kilonova heating rates
- \*separation energies for neutron capture and photodissociation rates
- \*impact neutron / gamma emission probabilities



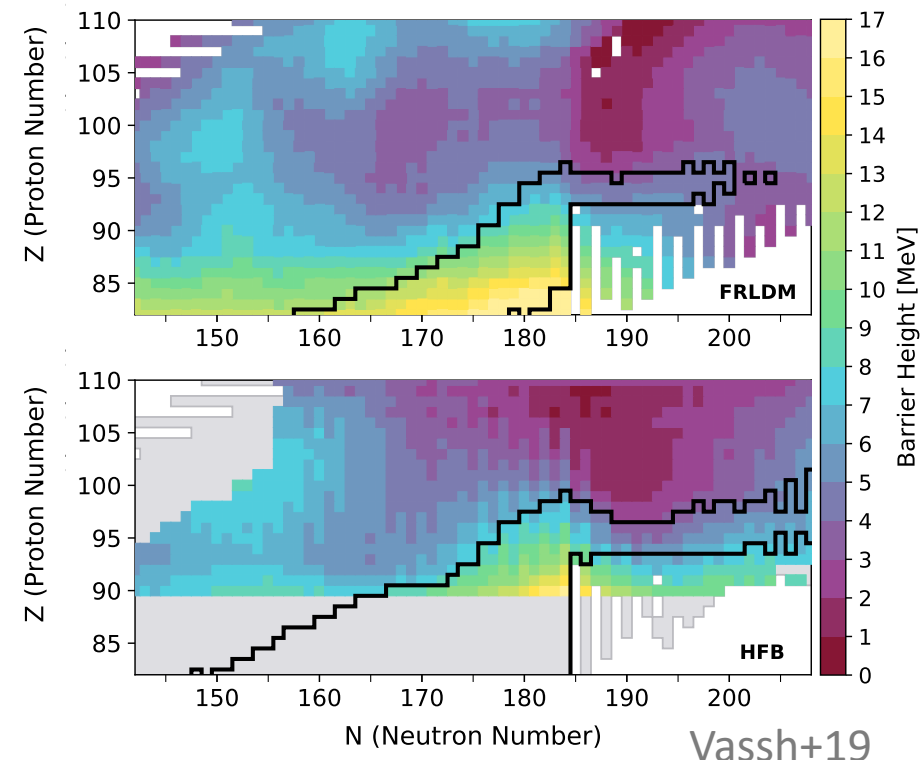
### Fission

- \*rates: neutron-induced,  $\beta$ -delayed, and spontaneous fission can impact abundances / EM signals as well as answer the big questions of termination and production of superheavy elements
- \*yields: especially important for interpreting *r*-process enhanced, metal-poor star abundances
- \*neutron and gamma emission: gammas > 3.5 MeV distinct to fission

adapted from Vassh+21



Vassh+20

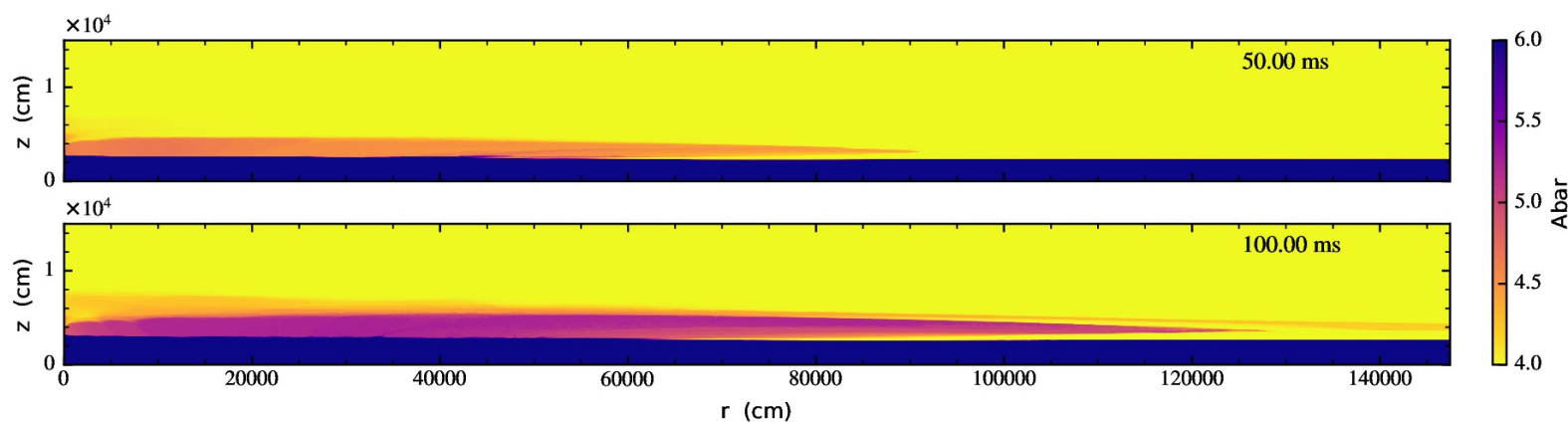
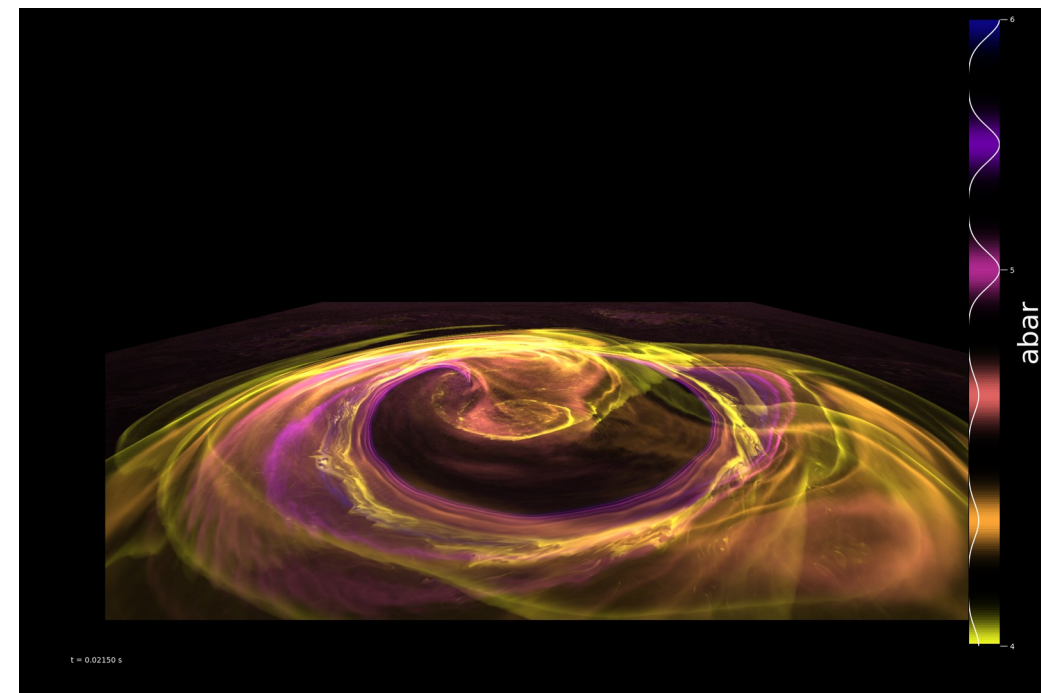


Vassh+19

# X-ray bursts

## What Are We Doing?

- Our focus has been on resolving the structure of the flame and using realistic nuclear physics
  - GPUs essential for these simulations
  - Both H/He and pure He bursts
  - Magnetic fields soon



▲ 3D simulation of He flame spreading across the surface of a neutron star (Zingale et al. In prep)

◀ 2D simulation of He flame on neutron star (Harpole et al. 2021)

# Future Goals

- A longterm goal of XRB modeling is to accurately capture the nuclear physics in a full-star model of the spreading of the flame
  - Will require a subgrid model
  - May require true multiscale methods (e.g., different approximations at different resolutions)
- Lightcurve modeling of multidimensional explosion



# Next decade: “Golden Age” of Neutron Stars

We might pin down the **equation of state**, the existence of **phase transitions** to exotic forms of matter, and we might reliably constrain **microscopic interactions** (Hamiltonians) between fundamental particles!

## Theory:

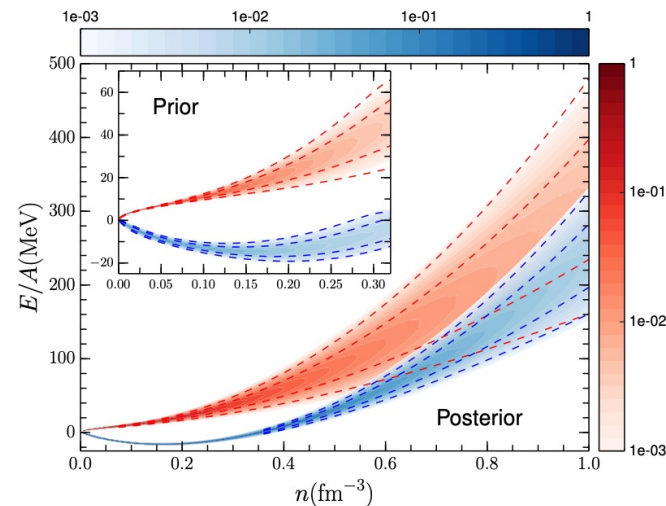
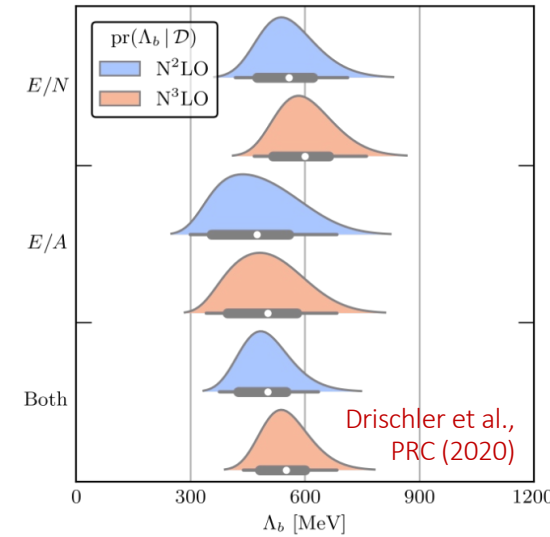
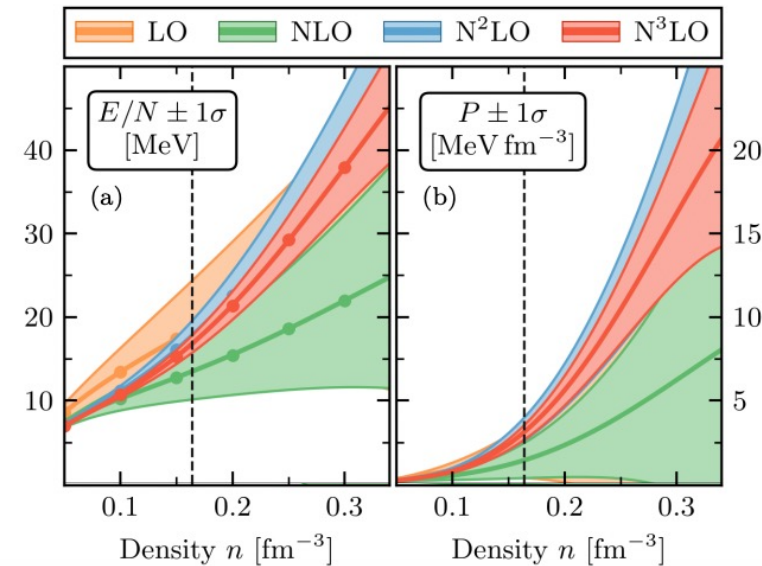
- **“low” densities:** Combine chiral EFT plus modern computational tools (machine learning, emulators, Bayesian inference) for more precision, uncertainty quantification, answer open problems in EFTs (regularization, convergence, ...):

At which densities and how does the EFT description of nuclear matter break down?

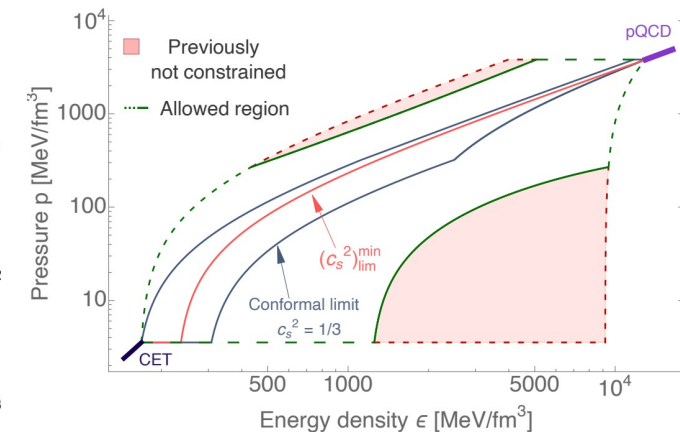
- **“High” densities:** Perturbative QCD might constrain EOS at neutron-star densities, but how robust, how far down in chem. potential is this approach reliable?

- **In-between:** Currently, general approaches (polytropes, speed of sound, Gaussian processes) used in analyses, but we need microscopic models with UQ:

If we constrain the EOS, what does this imply for the microphysical degrees of freedom?



Lim & Holt, PRL (2018)



Komoltsev & Kurkela, PRL (2022)

# Next decade: “Golden Age” of Neutron Stars

We might pin down the **equation of state**, the existence of **phase transitions** to exotic forms of matter, and we might reliably constrain **microscopic interactions** (Hamiltonians) between fundamental particles!

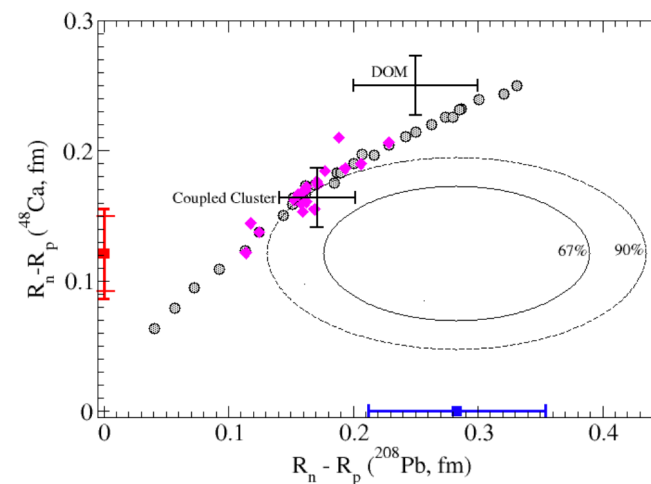
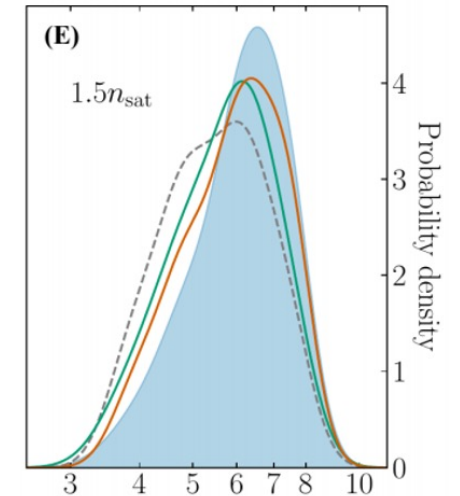
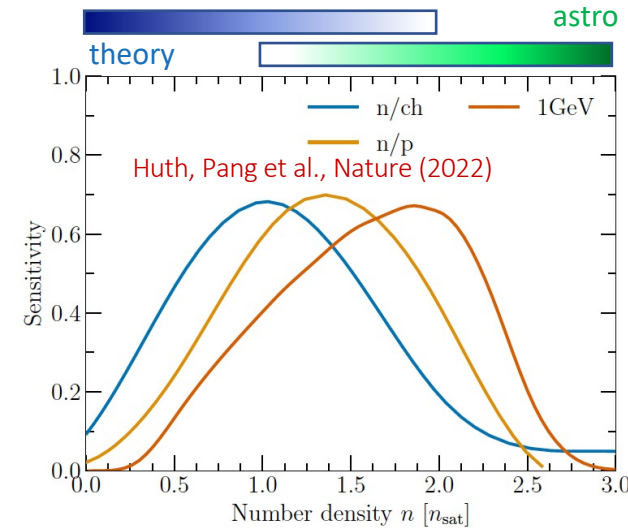
## Experiment:

- **Heavy-Ion Collisions:** Provide benchmarks and bridge between densities where theory and observation are most sensitive! But uncertainties need to be reduced.

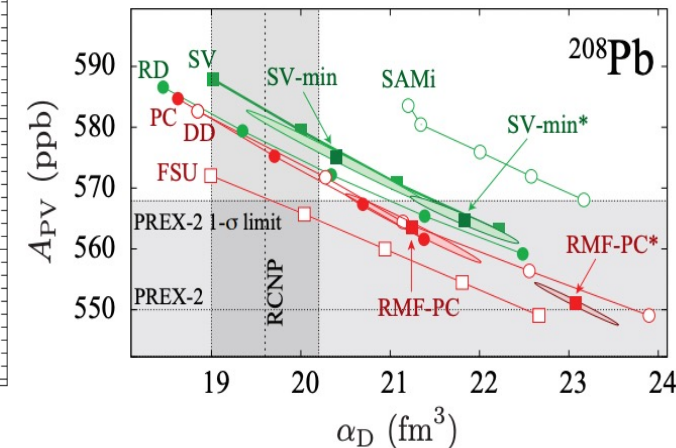
How can HIC experiments be maximally useful to constrain the EOS?

- **Neutron-Skin Thickness:** Slight “tension” between CREX and PREX results and between PREX and dipole polarizability. There needs to be coherent effort that considers all available experimental data and their uncertainties.
- PREX prefers a stiff symmetry energy. If confirmed (e.g., by MREX) this provides strong constraint for EFTs. But will uncertainties be small enough for such a challenge?

Which features would theoretical models need to have to comfortably describe both PREX and CREX? What is their impact on the EOS? How does this affect *ab initio* theory?



CREX collaboration, PRL (2022)



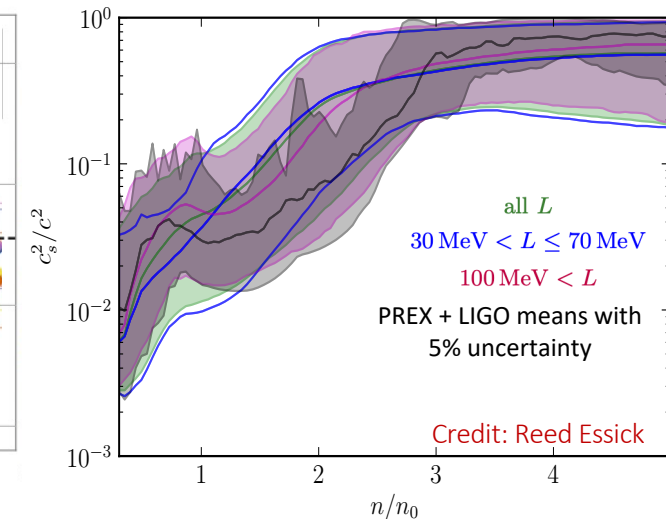
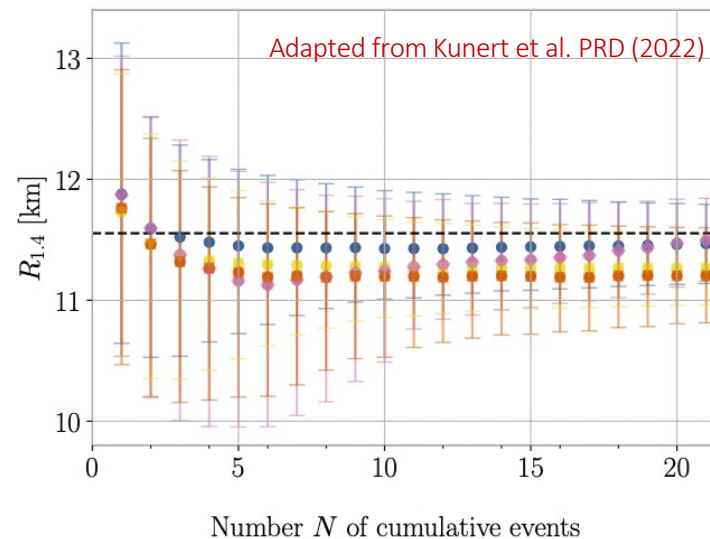
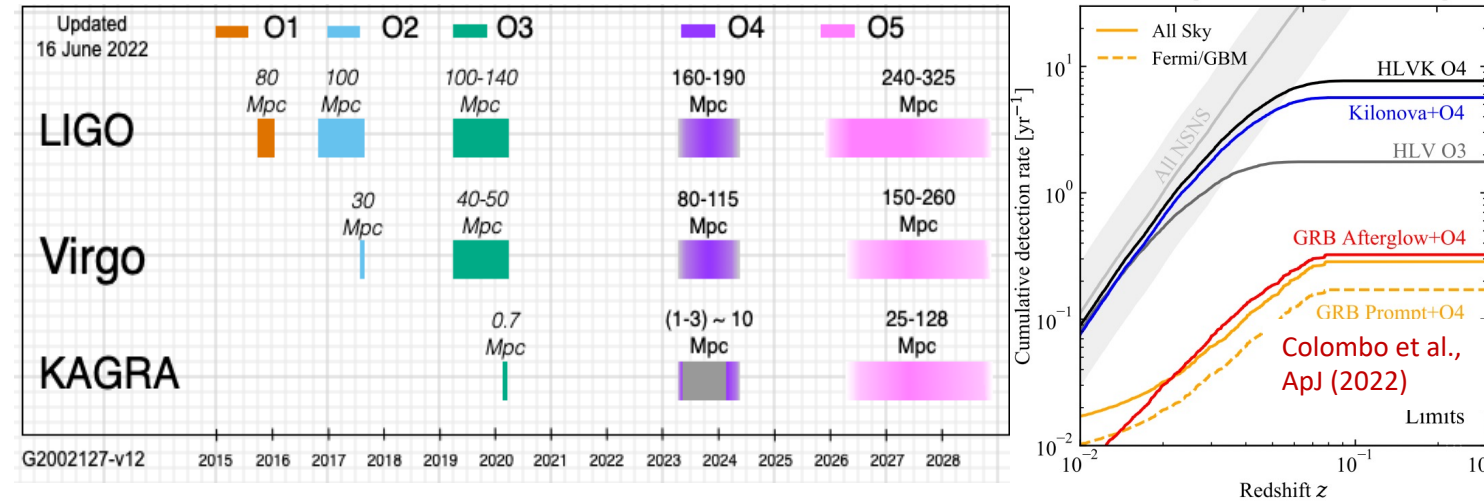
Reinhard et al., PRL (2021)

# Next decade: “Golden Age” of Neutron Stars

We might pin down the **equation of state**, the existence of **phase transitions** to exotic forms of matter, and we might reliably constrain **microscopic interactions** (Hamiltonians) between fundamental particles!

## Observation:

- **Gravitational Waves:** In O4, LIGO might observe 3 (more pessimistic) to 7 (reasonably optimistic) neutron star mergers, maybe a few with kilonova.
- No postmerger signal unless event very close (within 20 Mpc). Maybe we get lucky (again)?
- **Electromagnetic observations:** Kilonova observations are crucial to probe physics at highest densities (without postmerger GW signal), we need detailed astrophysical modeling of these events.
- EM observations by NICER (extended for 3 years), eXTP, etc. will provide additional data.



What are observational signatures of exotic microphysical d.o.f. in the core of neutron stars?

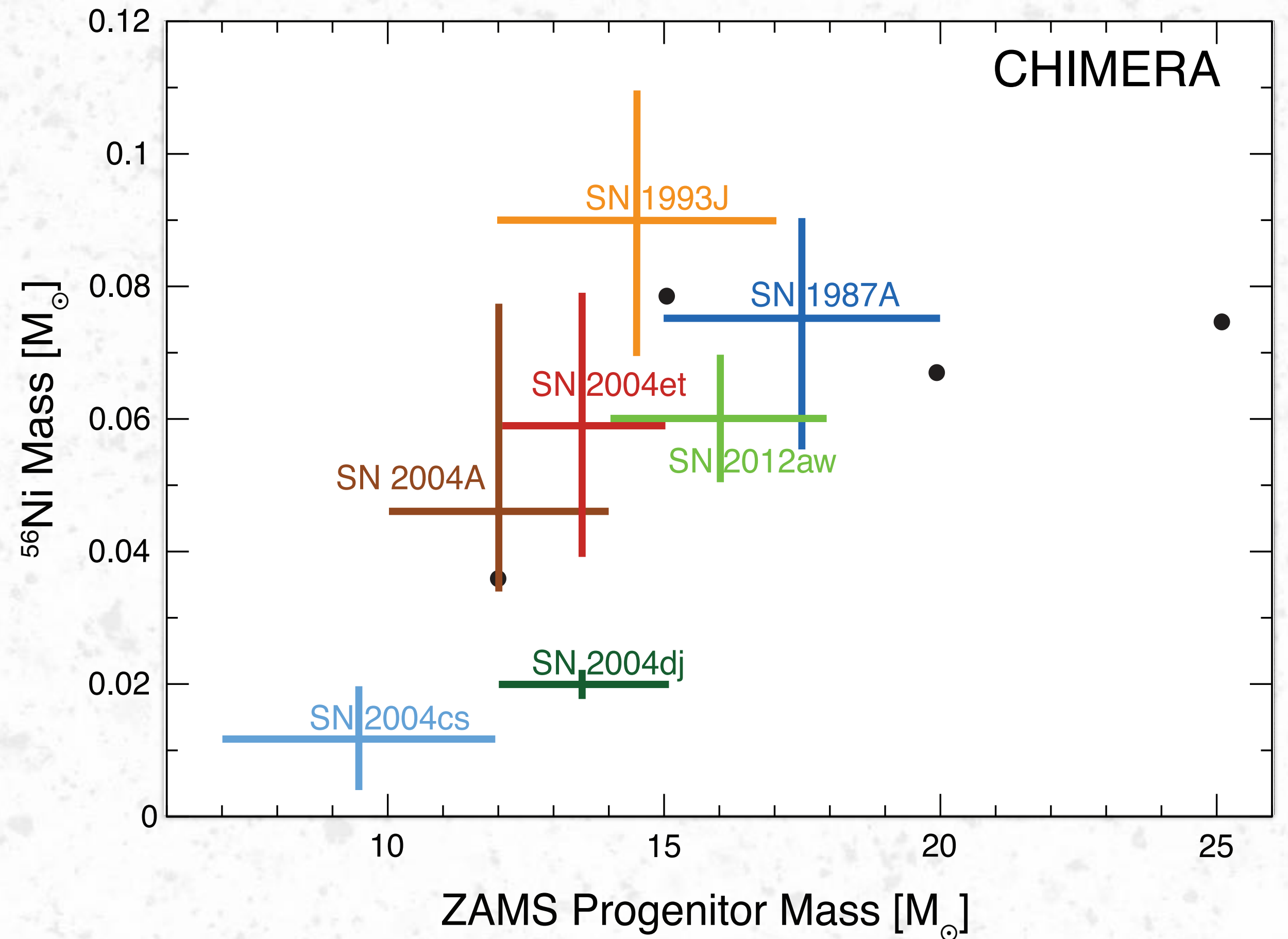
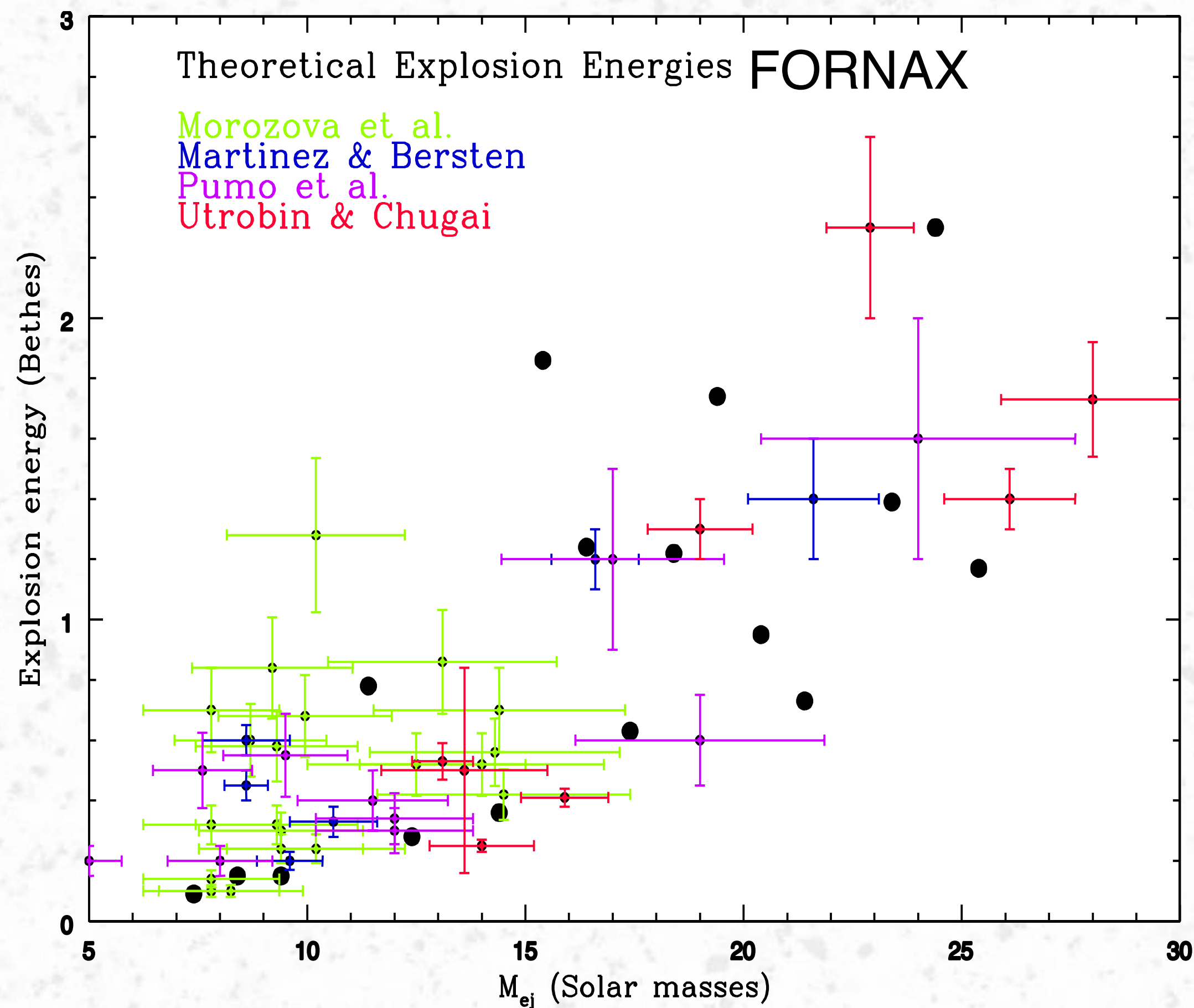
How can we foster interdisciplinary, multiphysics analyses of these and other data?

# PAST DECADE'S CCSN PROGRESS

In the past decade, we've achieved qualitative agreement with basic observables.

Requires simulations with spectral neutrino transport and (approximate) GR.

Also requires continuing models for several seconds (more for higher masses).



# NEXT DECADE'S CCSN PROMISE

1) Compare to quantitative observations.

Requires detailed nucleosynthesis

Requires end-to-end simulations

2) Understand how details of stellar structure, stellar generation and binarity manifest in supernovae.

Requires more models

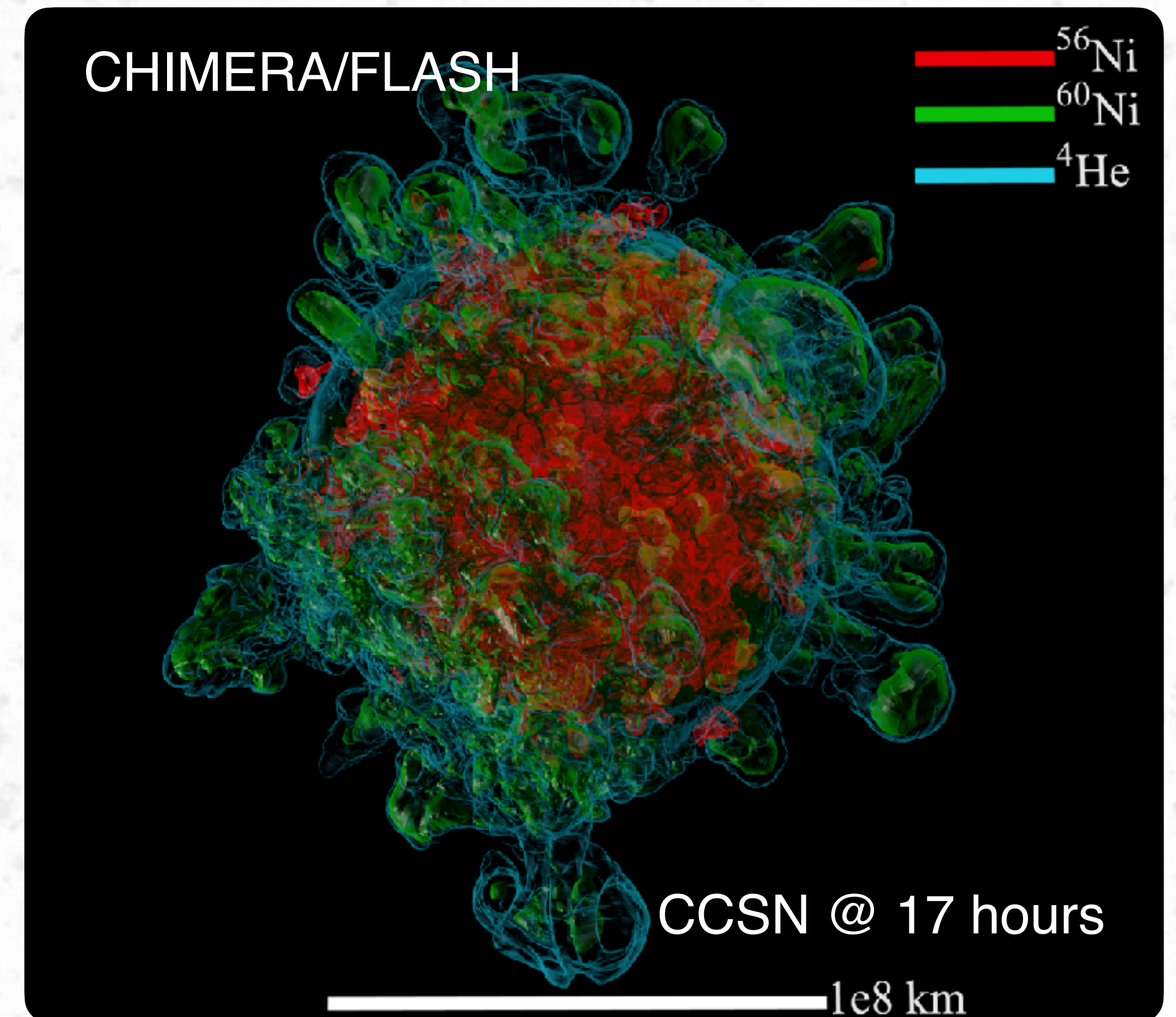
3) Model the full massive star menagerie:

Long GRBs with SN, SN that form

Magnetars, Electron-Capture SN, Super-

luminous SN and new things Vera Rubin (Telescope) will find.

Requires better physics (neutrino oscillations, full GR, better Equation of State and neutrino opacities, ...)

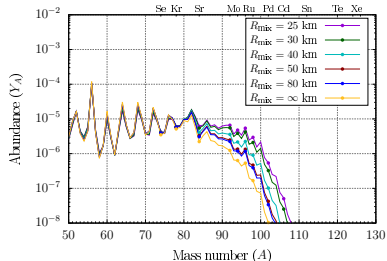
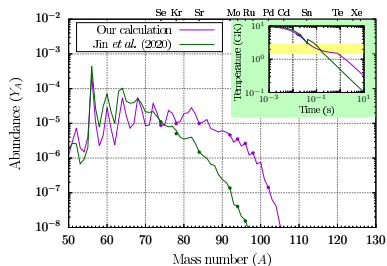


# MULTI-MESSENGER THEORY

To compare to all of the observations, we must building a continuous chain of core-collapse supernova/remnant simulations linking the earliest moments of the explosion, when the neutrino & gravitational wave signals originate, to the epochs when the nucleosynthesis is revealed.

1. Need to examine late stellar evolution in multi-dimensions.
2. Need to model CCSN mechanism with 3D spectral neutrino radiation hydrodynamics and detailed nucleosynthesis until the explosion matures and the nucleosynthesis finishes.
3. Need to model progress of the shock and heavy element ejecta through the star.
4. Need to model shock breakout and the light curve phase with (3D?) photon radiation hydrodynamics, etc.
5. Need to model nebular phase with full chemistry, etc.
6. Need to model supernova remnant phase including cosmic ray generation, etc.

Need seamless hand-off between each of these stages.



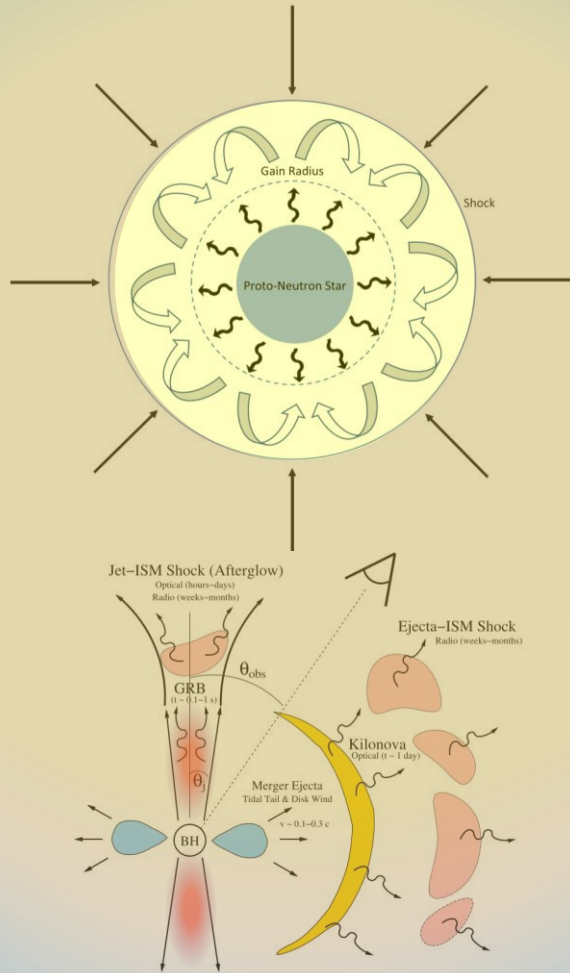
Effect of hydrodynamics (top) and neutrino flavor mixing (bottom) on the  $\nu p$ -process



Physical inputs into the  $\nu p$ -process, and the path forward for establishing its viability in accounting for solar system abundances of relevant nuclides.

# Flavor Transformation

- Vacuum (easy)
- MSW (easy)
- Collective Oscillations
- Matter-Neutrino Resonance
- Halo Effect
- Fast Flavor Instability





# How to span the full dynamic range?

Need all four approaches to connect large to small scales in a controlled way

reduced coupling

Global features, artificial scaling  
6 flavors, ~1m resolution in some tests  
1 postdoc year per code?

effective models

Global features, discard information  
6 flavors, inexpensive model by design  
1 grad student year ONCE models exist

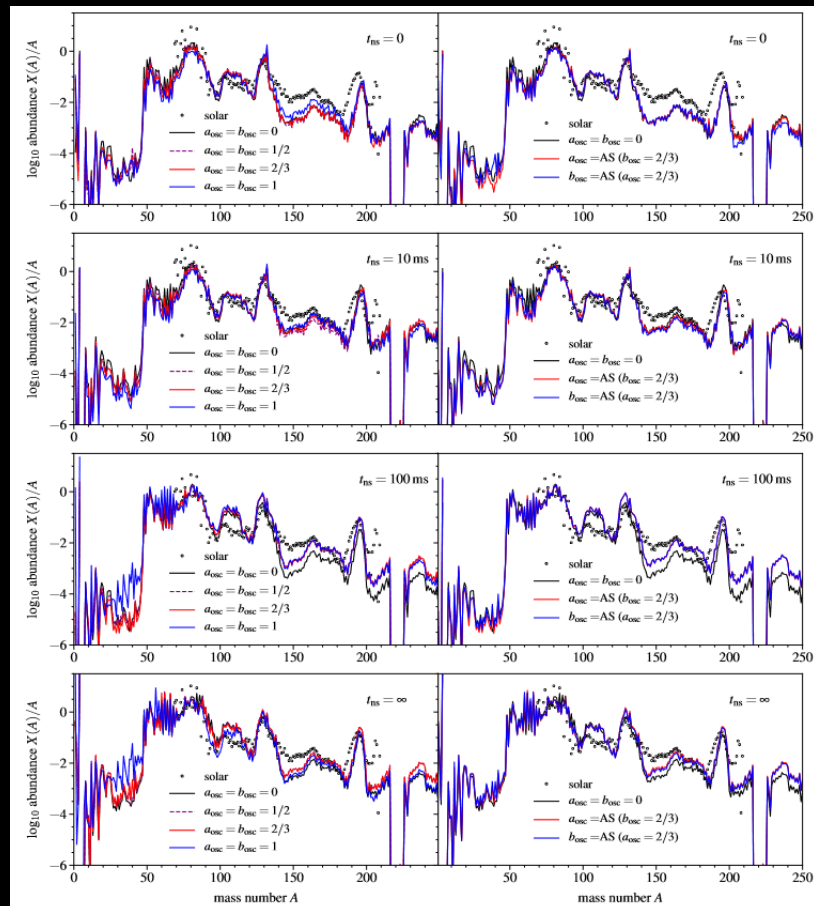
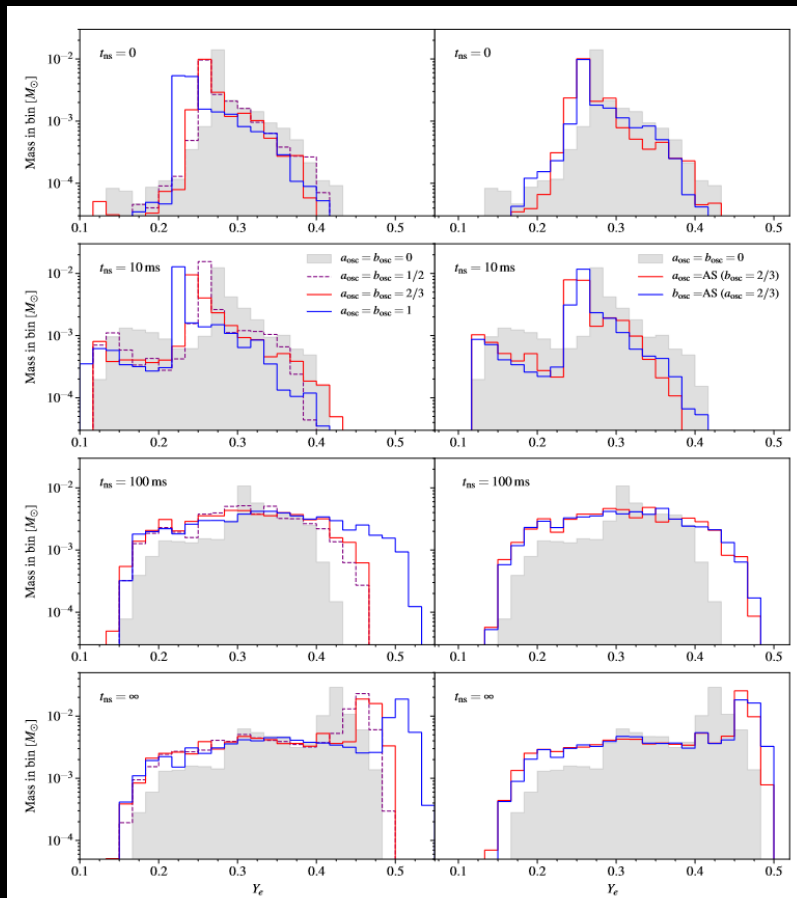
exact toy models

Exploring phenomena  
Minor computational cost  
Check on every approximation

easier equations

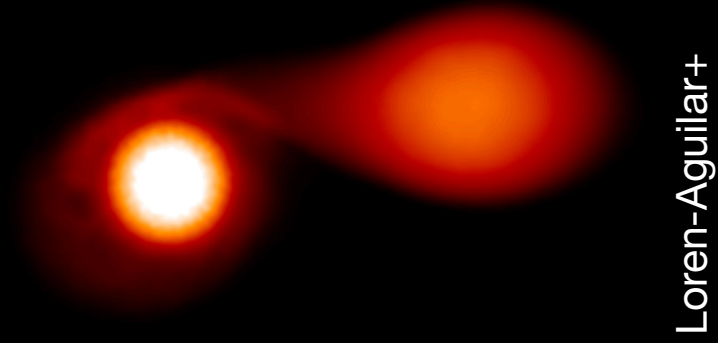
Global features, discard information  
6 flavors, likely use w/ reduced coupling  
1 postdoc year per code?

# Expect FFI to have a moderate impact on outflows



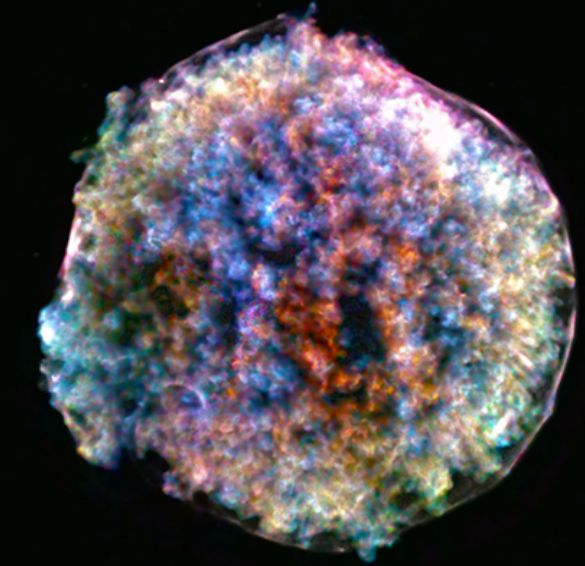
# Modeling SNe Ia/x Transients

Stellar/Binary Evolution  $10^8 \text{ yr} - 10^{10} \text{ yr}$



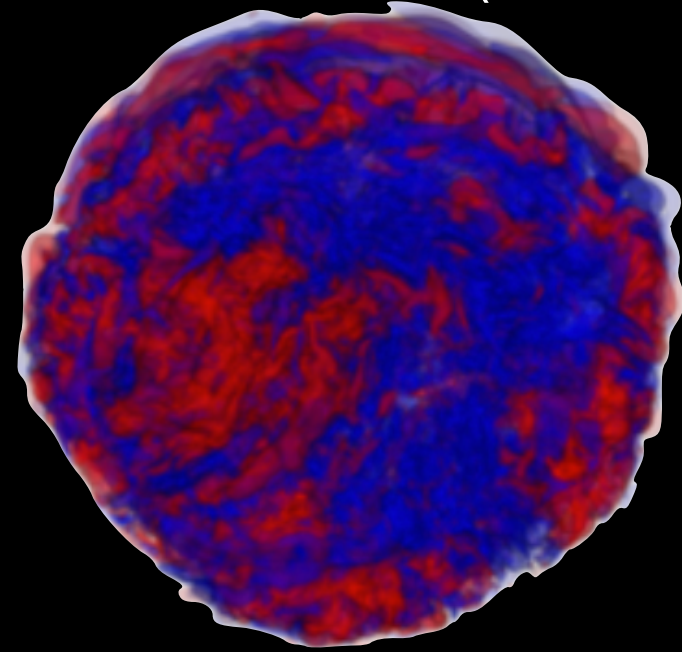
Loren-Aguilar+

Supernova Remnant  $10^2 - 10^3 \text{ yr}$



NASA CXG

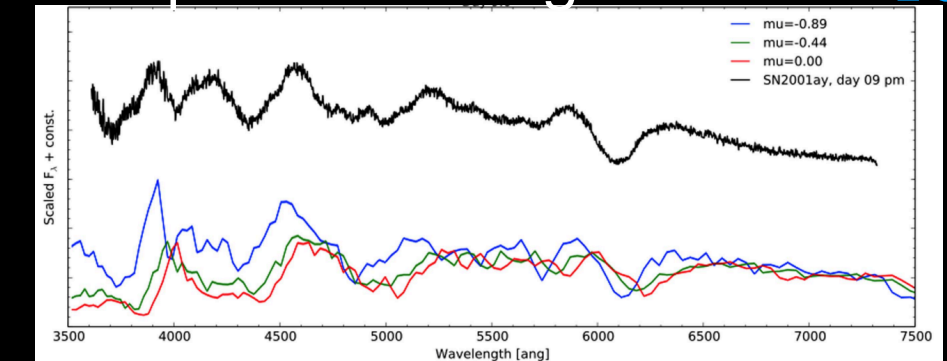
Smoldering Low Mach Number Hydro Simulations (Near- $M_{\text{Ch}}$ )  $10^2 \text{ yr}$



Zingale+

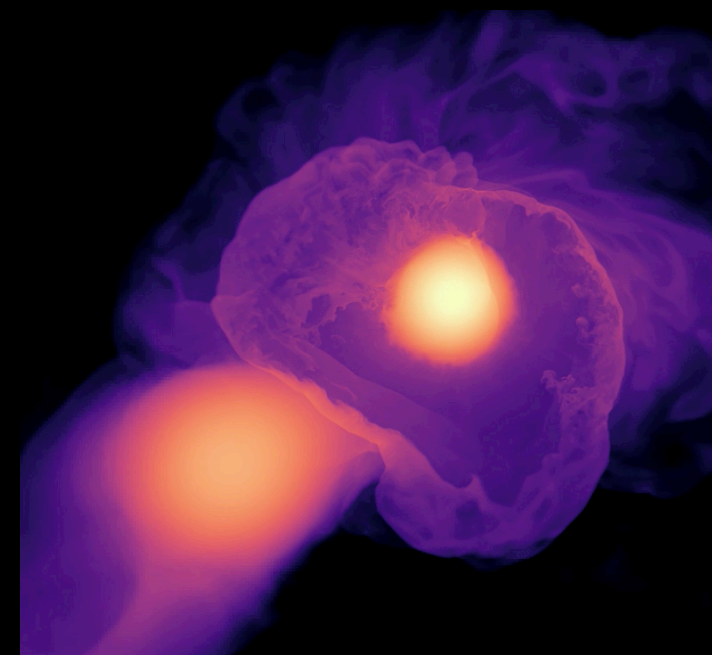


Nucleosynthesis + Synthetic Spectra and Light Curves  $10 - 10^3 \text{ d}$



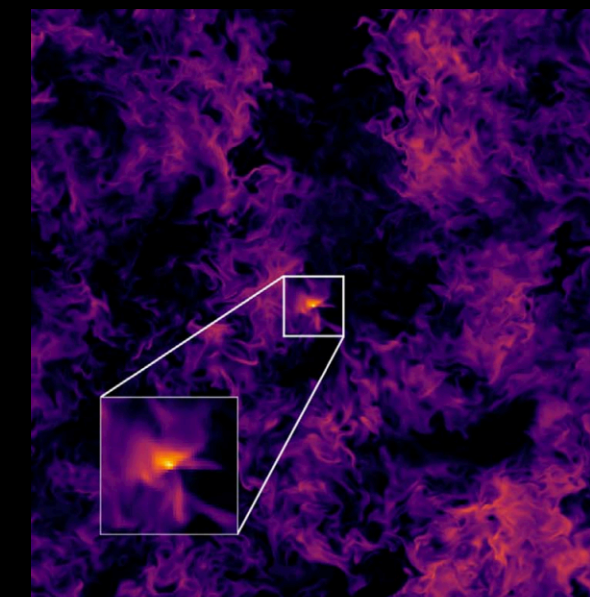
Van Rossum+

Multidimensional Hydro and MHD Simulations of Accretion and Merger  $1 - 10^3 \text{ s}$



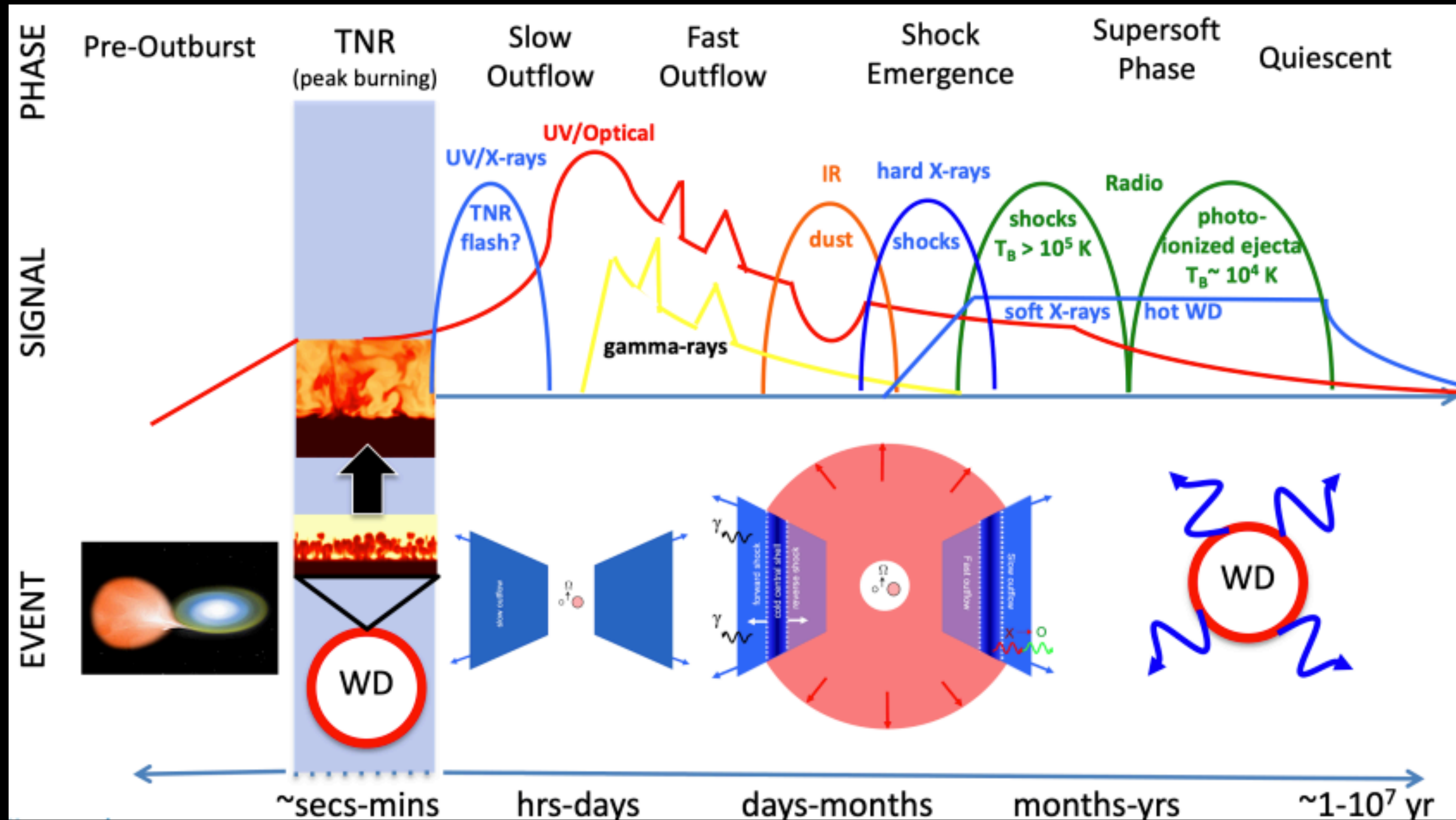
Roy+

Detonation Initiation  $10^{-9} - 10^{-3} \text{ s}$



Casabona+

# Modeling Classical Novae



# Progress Since Last NSAC Town Hall (NAP White Paper 2015 Strategic Directions)

Fisher

	Observational / Experimental Progress	Modeling Progress	Open Questions
SN Ia Progenitors (WD Explosions Direction1)	Gaia Hypervelocity WDs lax ex-companion LP 40-365	Helium-ignited mergers	$^{44}\text{Ti}$ probes helium burning
Convection and Detonation / Novae (WD Explosions Direction1)	Ubiquitous Nova GeV Emiss. Turb. Detonation Initiation	Low-Mach Number He Shells	Novae: A Grand Challenge? SN Ia/x Progenitors?
Nucleosynthesis, Synthetic Spectra and Light Curves (WD Explosions Direction2)	Constraints from 11fe, Gamma rays from 14J	Importance of non-LTE	Early Spectra, Bumps Stable Ni in Nebular Phase
SNRs	Absence of ex-companions 3C 397: near- $M_{\text{Ch}}$ SNR	3D Hydrodynamical Models 3C 397	Det. Mech. 3C 397?

# Network for Neutrinos, Nuclear Astrophysics, and Symmetries

*Multi-Messenger Nuclear Astrophysics  
Inner Space/Outer Space/Cyber Space Connectivity*

## **The goals of N3AS**

- focus on the field's big scientific challenges, ones requiring close coordination among theory teams
- do science that will increase the impact of new, \$1B-class instrumentation
- help a new generation of young theorists from our community acquire breadth they need to contribute to this multi-messenger, multi-physics field

## **History**

- proposed as a DOE Topical Collaboration in 2010, by UCB and UCSD
- funded as an NSF Physics Theory Hub in 2016
- enlarged to an NSF Physics Frontier Center in 2020

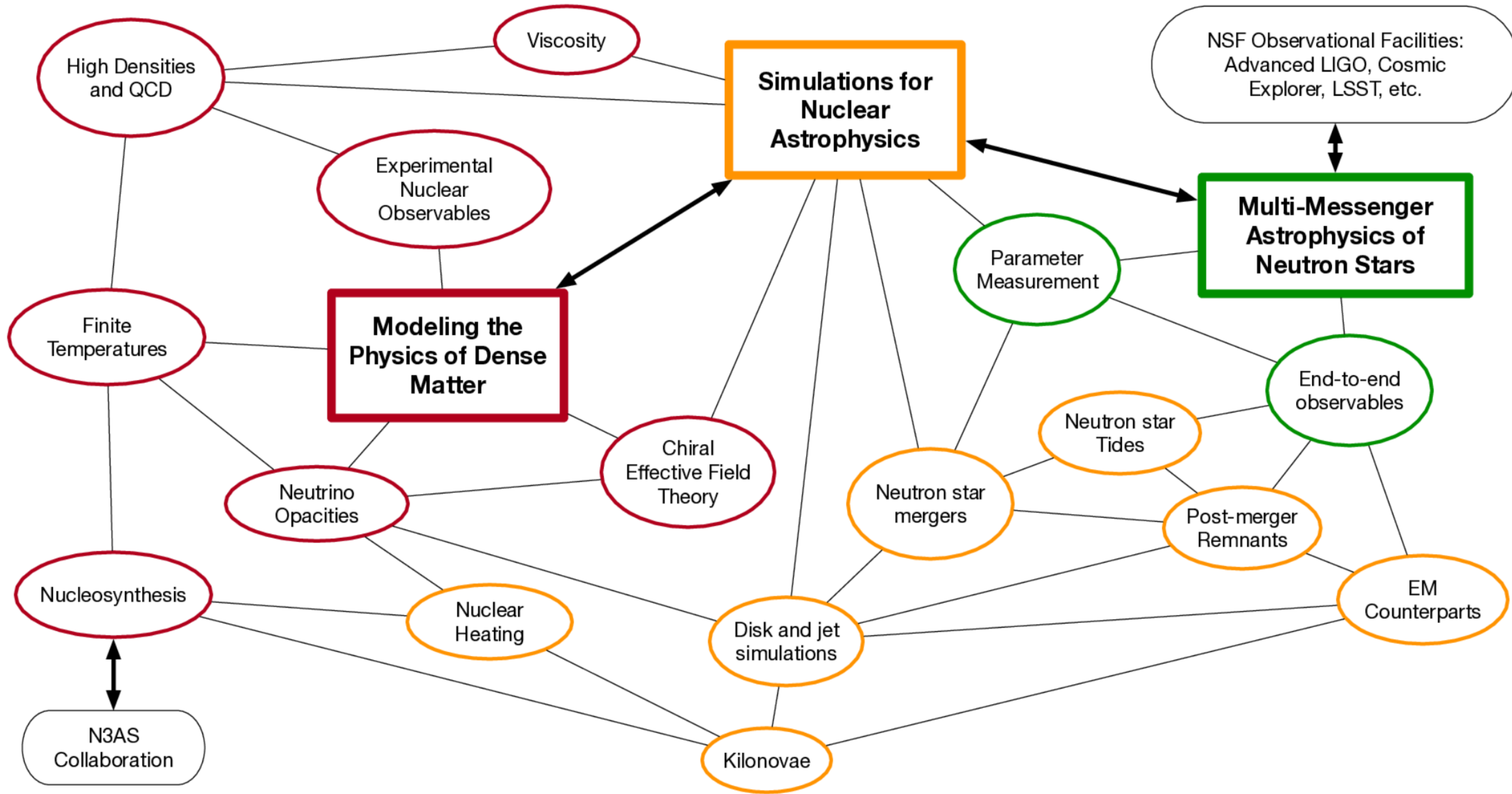
13 US University/Lab Partners  
RIKEN + CNRS  
Fully operational Fall 23





## Why NP3M?

- NSF Focused Research Hub
  - Nuclear physics of neutron star mergers
  - PIs: Duncan Brown, Chuck Horowitz, David Radice, Claudia Ratti, Andrew Steiner
  - Fellows: Peter Hammond, Zidu Lin, Rahul Somasundaram, Lami Suleiman (starting early 2023)
  - SIs: Veronica Dexheimer, Joshua Dolence, Joaquin Drut, Francois Foucart, Chris Fryer, Kathleen Hill, Raph Hix, Jeremy W. Holt, Davide Lazzati, Witold Nazarewicz, Ralf Rapp, Jocelyn Read, Srimoyee Sen, Rebecca Surman, Ingo Tews, and Ashley Villar
- End-to-end merger simulations with uncertainty quantification
  - Strong connection to GW community
  - Connections to RHIC Theory
  - Training early-career scientists
  - Hammond: High-resolution simulations of the MRI in the postmerger remnant and BNS merger simulations with MHD and neutrinos
  - Lin: Uncertainty quantification for neutrino opacities and the neutrino/GW signal of the SASI instability
  - Somasundaram: QMC calculations of the EOS using CEFT at N3LO and uncertainty quantification
  - Suleiman: Electron captures in an accreted neutron star crust and the impact of the crust-core transition on the GW signal





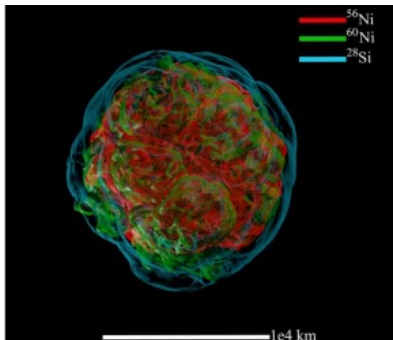
# ExaStar: Exascale Multi-Physics Simulations of Stellar Explosions

## ECP Team and Funding

- ECP Stakeholders: Total ECP funding: \$9.3M
- Core ECP Team Members

LBL	Kasen, Almgren, Wilcox, Peterson
ORNL	Messer, Endive, Harris, Hix, Mewes, Sandoval, Georgiadou
ANL	Dubey, Weide, Tzefaeracos, Graziani, Grannan, Chawdhary, O'Neal
Partners	Zingale (SUNY), Couch (MSU)

## Key Simulation Milestone



*3D core collapse supernova simulation evolved to shock breakout with Flash-X*

## ECP Challenge Problem

Multi-physics simulation of the post-bounce evolution of a core collapse supernova, including hydrodynamics, gravity, two-moment neutrino transport, and nuclear kinetics.

## Software Products Delivered

Core Modeling Capabilities	<ul style="list-style-type: none"> <li>Finite volume hydrodynamics on adaptive mesh grids, tabulated high-density equation of state, discrete Galerkin methods for two-moment radiation transport, multi-pole methods for gravity/</li> </ul>
Codes	<ul style="list-style-type: none"> <li>Flash-X, Castro</li> </ul>
Target Domains	<ul style="list-style-type: none"> <li>Nuclear Astrophysics</li> </ul>
Key Software Dependencies	<ul style="list-style-type: none"> <li>AMReX, Flang, HDF5</li> </ul>

## Post-ECP Funding

Targeted | NP theory funding, non-DOE sources

Current post-ECP funding gap: \$2M/year

## Exascale and Beyond

- Parameter surveys of 3D simulations that address the mechanism and diversity of stellar explosions, and link data from new nuclear experimental facilities with astrophysical observations of supernova signals
- Incorporation of dynamical spacetime solvers for modeling gravitational wave sources
- Maintain and grow code user-base

## Role of Multi-Institutional Centers

The importance of nuclear physics and related low-energy weak interactions to multi-messenger astrophysics is widely appreciated in physics.

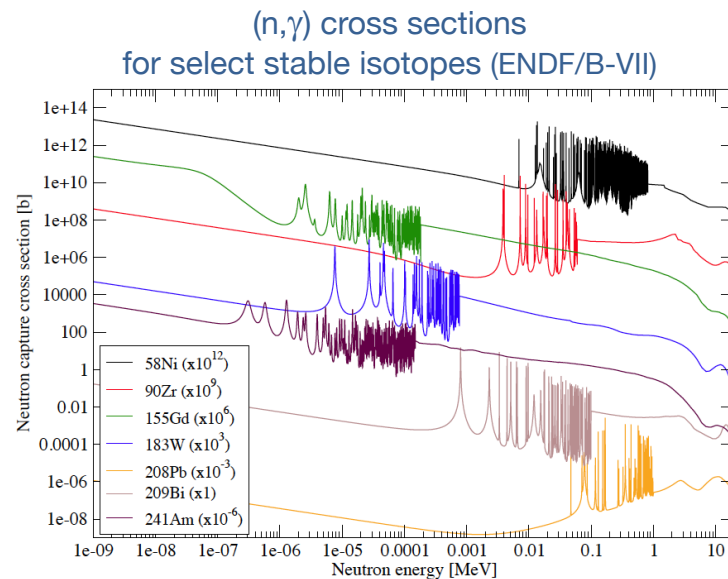
We can be successful in competition with other physics areas.

By competing for such centers, we have an opportunity to bring needed resources into nuclear astrophysics.

Good for us and important to progress in the science.

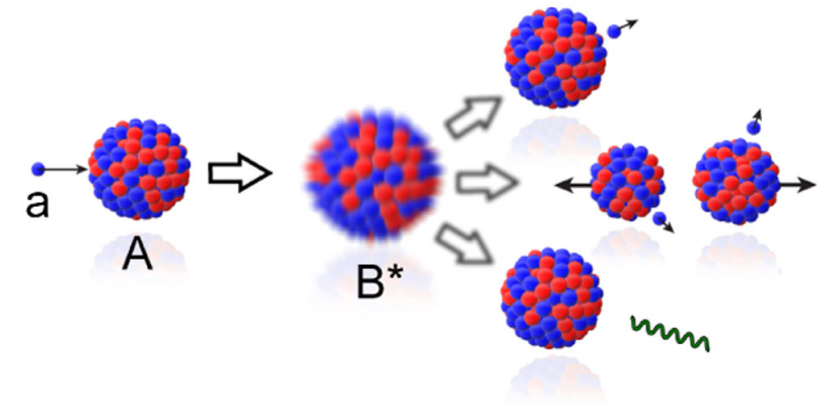
# We need to address the limitations of Hauser-Feshbach calculations

- Hauser-Feshbach (HF) reaction descriptions make an averaging assumption, which is not valid in all regions relevant to astrophysics - problems occur for low energies, closed shells, light nuclei, far from stability
- Data evaluators face related challenges: regions with too many channels for R-matrix analysis and level densities too small for statistical approach



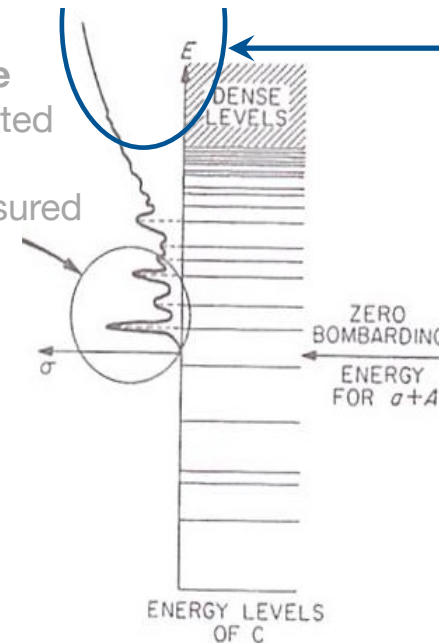
We need:

- Criteria for estimating the limits of validity for HF
- Usable prescriptions for treating compound reactions proceeding through isolated or weakly-overlapping resonances, bridge to HF
- Structure information for calculating direct-reaction contributions
- An assessment of uncertainties and experimental information



## R-matrix regime

- Assumes isolated resonances
- Requires measured data or fully microscopic calculation



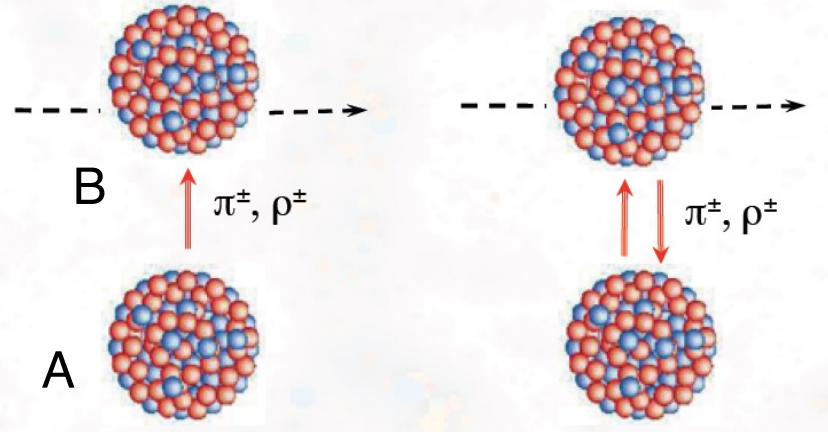
## Hauser-Feshbach regime

- Assumes strongly overlapping resonances
- Requires structure models and parameters

$$\sigma_{\alpha\chi} = \sum_{J,\pi} \sigma_{\alpha}^{\text{CN}}(E,J,\pi) \cdot G_{\chi}^{\text{CN}}(E,J,\pi)$$

\*WFC omitted here to simplify notation.

# Charge-exchange reactions & supernovae



One step

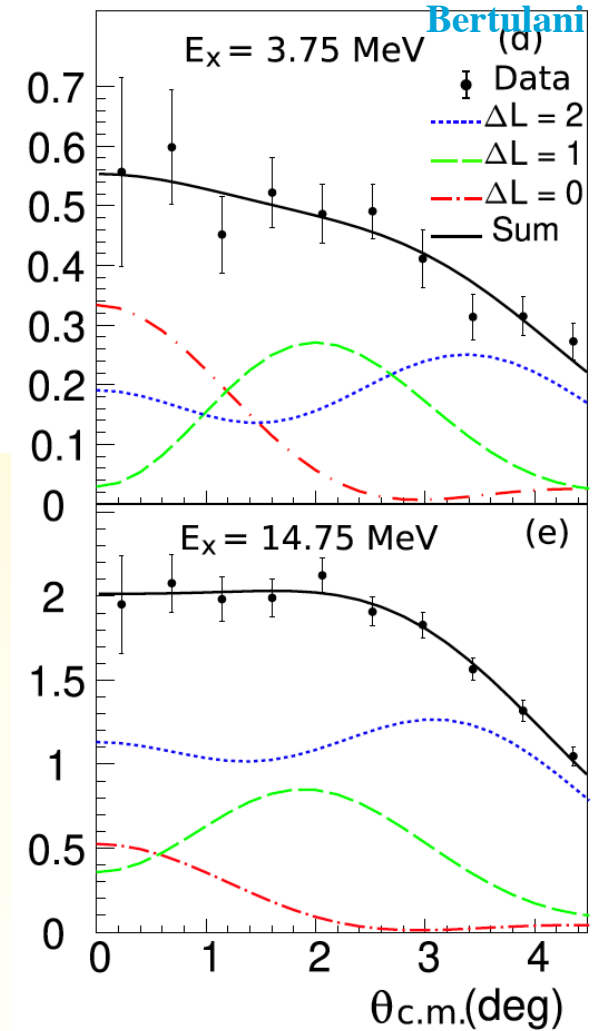
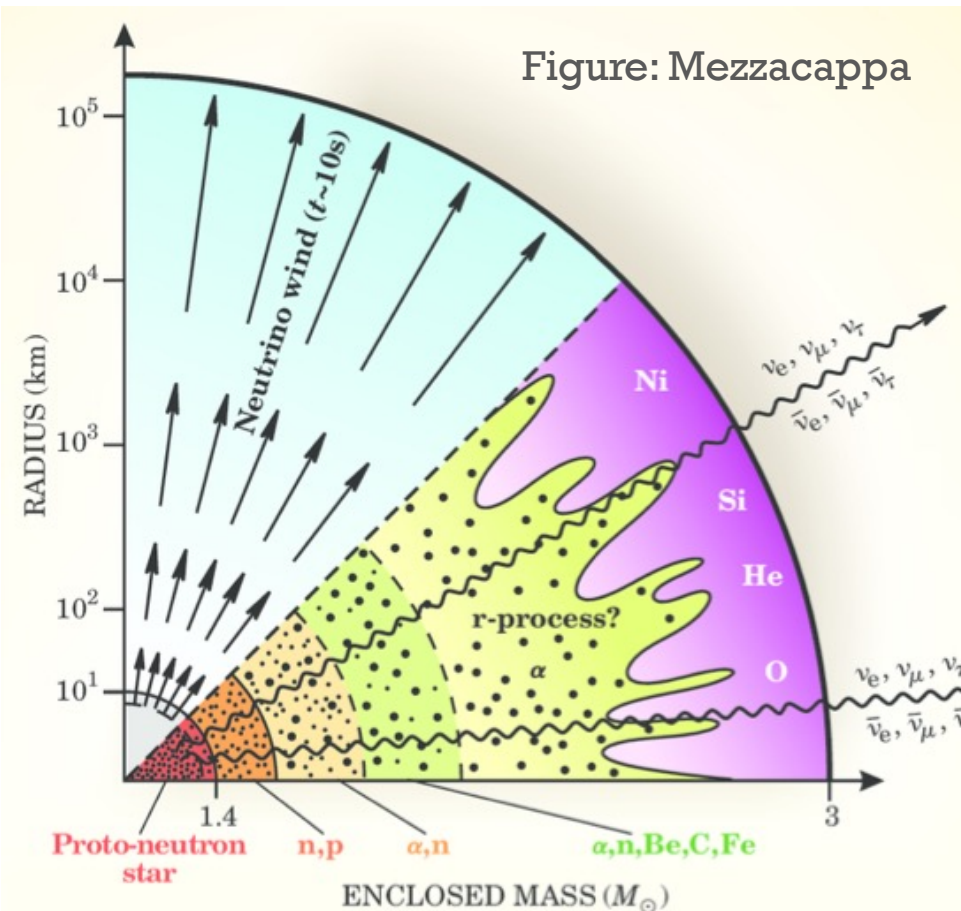
Two step  
(meson exchange)

(→ double-beta decay)

Applications to numerous electron capture  $e^- + (Z,A) \rightarrow (Z-1, A) + \nu_e$  and  $\nu$  induced reactions in supernovae

Fermi & Gamow-Teller ME read directly from exp.  $d\sigma/d\Omega(\theta \sim 0^\circ)$

More theoretical reaction studies needed on *optical potentials, relativistic effects, offshellness, factorization hypothesis, multistep reactions and medium effects*



Gao, et al, PRC (2020)

$^{93}\text{Nb}(t, ^3\text{He} + \gamma)$  at 115 MeV/A  
→ B(GT) in  $^{93}\text{Zr}$